

Shell-Model Monte Carlo Simulations of Pairing in Few-Fermion Systems

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(Dated: August 4, 2008)

We study a trapped system of fermions with an attractive zero-range two-body interaction using the Shell-Model Monte Carlo method. The method provides *ab initio* results in the low N limit where mean-field theory is not applicable. The energy and pairing properties are presented as functions of interaction strength, particle number, and temperature. In the interesting region where typical matrix elements of the two-body interaction are comparable to the level spacing of the trap we find large odd-even effects and signatures of shell structure. As a function of temperature, we observe the disappearance of these effects as in a phase transition.

PACS numbers: 03.75.Ss, 05.30.Fk, 21.60.Ka

The physics of ultracold atomic gases has been intensively pursued experimentally and theoretically in the last decade. Recently there has been great interest in strongly-interacting Fermi gases where Feshbach resonances allow the tuning of the two-body interaction. Studies of the transition from a dilute gas of fermionic atoms to a Bose condensate of molecules have therefore been possible in the laboratory [1, 2, 3, 4, 5, 6]. While studies of degenerate Fermi gases have mostly dealt with large atom numbers and wide traps, efforts have begun to trap only few (1-100) atoms in tighter traps [7]. Also, with the implementation of three-dimensional optical lattices, a low-tunneling regime can be reached with essentially isolated harmonic oscillators containing only a few fermions at each site [8]. This means that one can now explore few-body fermionic effects in trapped systems with scattering lengths that are comparable to the inter-particle distance and the trap width.

In this *letter* we report on a theoretical study of harmonically trapped fermions using the Shell-Model Monte Carlo (SMMC) approach. This method has been extensively used in nuclear physics to determine nuclear properties at finite temperature in larger model spaces than can be handled in normal nuclear shell-model diagonalization [9, 10]. In the SMMC the many-body problem is described by a canonical ensemble at temperature $T = \beta^{-1}$ and the Hubbard-Stratonovich transformation is used to linearize the imaginary-time many-body propagator $e^{-\beta H}$. Observables are then expressed as path integrals of one-body propagators in fluctuating auxiliary fields. The method is in principle exact and subject only to statistical uncertainties. For equal mixtures of two hyperfine states at low density, the interaction can be modeled with an s -wave zero-range potential. It thus belongs to the class of two-body interactions which is free

of sign problems in the SMMC [10]. We present here the first application of this many-body method to ultracold gas physics.

We study the usual zero-range pairing Hamiltonian

$$H = \sum_i \frac{p_i^2}{2m} + \sum_i \frac{1}{2} m \omega^2 r_i^2 + \sum_{[ij]} V_0 \delta(\vec{r}_i - \vec{r}_j), \quad (1)$$

where we sum over all particles i and $[ij]$ denotes a sum over fermion pairs with opposite internal states. The trap frequency is ω , and V_0 denotes the interaction strength. The SMMC method was originally set up to handle nucleons, and pairing problems have been extensively considered [11]. The spin symmetric ultracold Fermi gas can now be easily mapped onto a single spin 1/2 nucleon species [12], as the two-body interaction in the Hamiltonian corresponds to standard nuclear pairing.

Simple dimensional arguments reveal that the matrix elements scale as $1/b^3$, where $b = \hbar/m\omega$ is the oscillator length. It is therefore natural to redefine the interaction strength in terms of $V_0 = -g\hbar\omega b^3$, where g is a dimensionless strength measure. To relate V_0 to the s -wave scattering length, one needs to regularize the zero-range potential and consider the finite model space cut-off, as pointed out in [13]. Here we will adopt the treatment in [14] and renormalize through continuum low-energy scattering. The energy cut-off used can be written $E_c = \alpha^2 \hbar\omega$ with $\alpha^2 = N_{max} + 3/2$. This defines a relation between V_0 , a , and E_c , which can be written as $4\pi a/b = g/(\alpha g/2\pi^2 - 1)$. This gives the effective interaction strength needed for a model space with $N_{max} + 1$ major shell. The relevant parameter regime is expected to be where the natural energy scale, given by the level spacing $\hbar\omega$, is comparable to typical two-body matrix elements between the trap states at $T = 0$ (as a quantitative measure we use the $(1s)^2 - (1s)^2$ element). This

TABLE I: Energies (in units of $\hbar\omega$) calculated with the SMMC method for a trapped fermion gas with interaction parameter $g = 10$ calculated at temperatures (in units of $\hbar\omega$) $T = 1/6$ and $T = 1/5$ for different particle numbers N . The statistical uncertainty is given in parenthesis. HOSD denotes the non-interacting energies at $T = 0$.

N	HOSD	$T = 1/6$	$T = 1/5$	N	HOSD	$T = 1/6$	$T = 1/5$
2	3	2.60(1)	2.62(1)	12	32	29.8(2)	29.9(1)
3	5.5	5.12(1)	5.14(1)	13	35.5	32.8(4)	33.3(2)
4	8	7.31(1)	7.37(1)	14	39	36.4(3)	36.6(2)
5	10.5	9.73(2)	9.76(1)	15	42.5	39.8(2)	39.9(2)
6	13	11.9(1)	11.9(1)	16	46	43.0(2)	43.1(2)
7	15.5	14.2(2)	14.3(1)	17	49.5	46.3(2)	46.5(2)
8	18	16.3(1)	16.4(1)	18	53	49.5(2)	49.7(2)
9	21.5	19.8(1)	19.9(1)	19	56.5	52.9(2)	53.1(2)
10	25	23.1(2)	23.2(1)	20	60	56.1(2)	56.4(1)
11	28.5	26.5(2)	26.6(1)				

turns out to be around $g \sim 10$ in our setup, which corresponds to $a = 10.66b$. The different regions of interest in terms of interaction strength and $\hbar\omega$ in the context of atomic gas physics are discussed in [15, 16]. We note, however, that our procedure to relate g and a is only approximate and modifications to the simple relation we use can occur, e.g. in tight traps [31].

Previous works have considered few-fermion systems using advanced many-body methods. The Green's function Monte Carlo methods were applied to homogeneous [17], as well as trapped systems [18]. No-core [19], and traditional shell-models [20], using effective interactions have also recently been applied to these systems, particularly for very low particle numbers where exact results are available [21, 22]. Finite-temperature, non-perturbative lattice methods have also been applied to homogeneous [23] and trapped fermions [24]. These works focus on the unitary $|a| \rightarrow \infty$ limit and the crossover regime around it. The present SMMC approach is not variational, but an exact many-body method subject only to statistical uncertainties. Our choices of N_{max} and g discussed above imply that the SMMC results given here are on the BEC side of the crossover regime.

In Tab. I we present the SMMC energies for two different temperatures small compared to $\hbar\omega$, along with the non-interacting energies. There is agreement between the two SMMC calculations within the uncertainties for almost all particle numbers. Notice that the absolute energy uncertainty decreases with increasing T , as expected [10]. The $N = 2$ problem can be solved exactly for all a [26], and with $a = 10.66b$ we find 2.4 for the $T = 0$ ground-state. Our value of 2.6 at $T = 1/6\hbar\omega$ thus indicates that we are close to the $T = 0$ limit. In general, we find that our energies are typically above those calculated at unitarity in [18, 21] and in the crossover regime in [25]. This is expected due to finite temperatures and

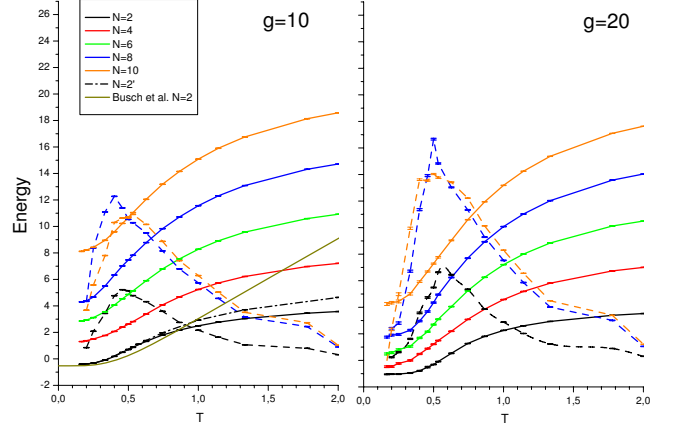


FIG. 1: (color online) The temperature dependence of the SMMC energies (both in units of $\hbar\omega$) for selected even N systems and for strength parameters $g = 10$ (left) and 20 (right). The zero-point energies are subtracted. Statistical uncertainties are too small to show. The dashed curves give the specific heat for $N = 2, 8$, and 10. Also shown are the exact $N = 2$ results (Busch *et. al.*, [26]) with $a = 10.66b$ for the full space. The dash-dotted curve $N = 2'$ gives the SMMC results for 5 major shells with $g = 8.98$.

also because of Hilbert space differences (see discussion below).

Fig. 1 shows the SMMC energies as a function of temperature for selected even particle numbers and for the strength parameters $g = 10$ and 20. We can clearly see the convergence of our results at small T , approaching the $T=0$ ground state value. Quantitatively we find that the energies increase by about 1% (2%) going from $T = \hbar\omega/6$ to $T = \hbar\omega/5$ ($T = \hbar\omega/4$). At high T , the curves flatten out as they approach the equipartition limit of equal occupancies in the finite model space.

We have used moderately small model spaces of 4 major shells for most calculations, which might be problematic when using zero-range interactions. However, to check our convergence we have repeated the calculation for $N=2$ in an enlarged model space of 5 major shells with the interaction strength readjusted to the same scattering length parameter. As can be seen in Fig. 1 the two calculations, performed for $g = 10$ for $N_{max} = 3$ and $g = 8.98$ for $N_{max} = 4$, agree within the statistical uncertainty up to a temperature $T \approx 0.7$. We also compare our SMMC results with the exact solution of the $N=2$ system as given in Ref. [25]. The comparison, although quite reasonable at low temperatures, can only be indicative as the pseudopotential used in [25] is similar, but not identical to the present delta interaction and allows for a 2-body $1/r$ bound state which our calculation does not include. At large T , the energy expectation value approaches $E(T) = 3Nk_B T$ in the full model space. This behavior is, however, not obtained in our restricted

spaces where $E(T)$ converges to the thermal equilibrium values which are 4.5 and 6 for $N_{max} = 3$ and 4, respectively.

The $g = 10$ results show a sharp increase in the energy around $T \sim 0.3$. Correspondingly the specific heat $C = dE/dT$ exhibits a distinct peak around this temperature. Such a peak in the specific heat is usually associated with phase transitions in finite systems and indicates that the system changes its character. For $g = 20$ we see the peak at higher T as expected. As we will show below, it can be interpreted as the analogue of the superfluid-to-normal phase transition in finite nuclear systems [27, 28] and is associated with the breaking of pairs. Notice in particular that the peak height is larger for $N = 8$ than $N = 10$. This is a result of the shell closure at $N = 8$ which causes the energy to be released in a smaller interval as T increases. The sizable width of the peak is due to the finite size of the system. The model space discussion above demonstrates that our peaks are genuine and not a finite size Schottky effect [10].

To relate the peak in the specific heat to changes in the pairing correlations, we have calculated the expectation value of a number-conserving BCS-like pair matrix

$$M_{\alpha,\alpha'} = \langle \Delta^\dagger(j_a, j_b) \Delta(j_c, j_d) \rangle, \quad (2)$$

with the $J = 0$ pair operator

$$\Delta^\dagger = \frac{1}{\sqrt{1 + \delta_{ab}}} \left[a_{j_a}^\dagger \times a_{j_b}^\dagger \right]^{JM=00} \quad (3)$$

where $a_{j_a}^\dagger$ creates a particle in orbit j_a (which is the combination of orbital and spin angular momentum of the fermions). This operator is thus a measure of the pairs with $J = 0$. An indication of the pairing correlations can be obtained from the sum over all matrix elements, called pairing strength in the following [29]. Since we are only interested in genuine pair correlations we subtract the 'mean-field' values obtained at the same T but with $g = 0$.

In Fig. 2 we show the pairing strength as a function of particle number for different temperatures. The most striking feature is naturally the odd-even staggering. The relative reduction of pairing strength for odd-particle numbers is related to the blocking of scattering of pairs into the orbital occupied by the unpaired particle. The non-interacting systems have closed-shell configurations for $N = 2, 8, 20$. With interaction switched on, these configurations manifest themselves by a relative reduction of the pairing strength (overlaid by a general increase due to a growing number of pairs) and a larger resistance against temperature increase. The strong dips observed for particle numbers $N = 7, 9$ and 19 are also related to the shell closures. Relatedly the pairing strength is largest for mid-shell systems. From the inset we see that the staggering is larger for $g = 20$ and persists to larger temperatures as expected.

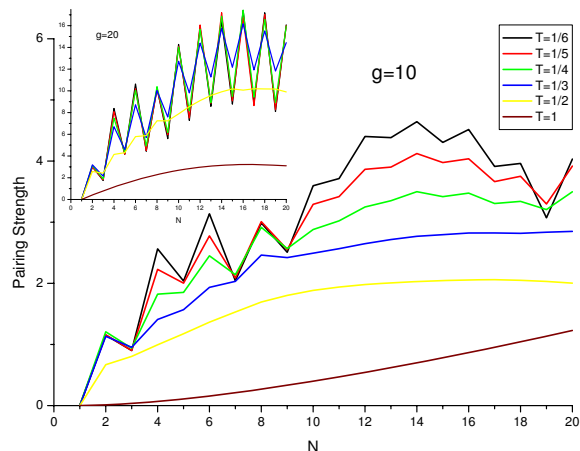


FIG. 2: (color online) The pairing strength as a function of particle number, N , for various temperatures, T (in units of $\hbar\omega$) for $g = 10$. The upper left inset shows the results for $g = 20$. The uncertainties are very small and not shown.

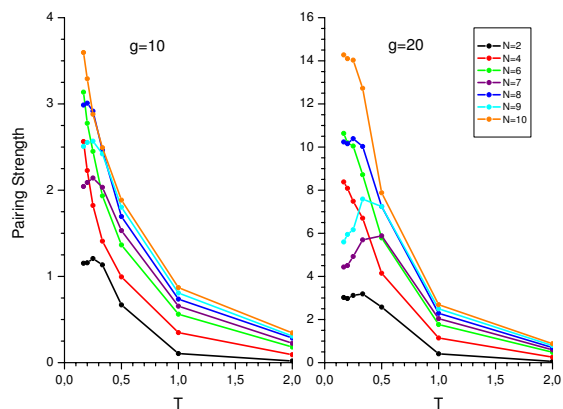


FIG. 3: (color online) The pairing strength as a function of temperature, T (in units of $\hbar\omega$), for various particle numbers, N and for $g = 10$ (left) and $g = 20$ (right). Uncertainties are small and not shown. Note the different scales in the two panels.

As function of temperature, the pairing strength for $g = 10$ decreases and the odd-even effects vanish around $T \sim (1/3 - 1/2)\hbar\omega$ except for the lowest N . This is consistent with the value at which the energies show sharp increases in Fig. 1 with resulting peaks in the specific heats. The same is seen for the $g = 20$ results. At higher T we see only a monotonous increase with N , indicating equipartition in the model space with loss of all shell structure.

To investigate further the transition between a paired state and a normal state, we show the pairing strength for $g = 10$ and $g = 20$ as a function of T for selected particle

numbers in Fig. 3. We note that the pairing correlations decrease rapidly for all particle numbers in the temperature regime which corresponds to the peak structure in the specific heat (with the strong decrease happening at larger T for $g = 20$ as expected). We have calculated the pairing strength up to $T = 4$, at which point it has practically vanished for all N . We believe this indicates that the transition temperature for our low particle numbers is some numerical factor less than unity (depending on g and N) times the trap spacing $\hbar\omega$. Notice how the closed shell numbers $N = 2$ and 8 have different low- T behavior from the other systems (also the case for $N = 20$ which is not shown). Here the pairing remains relatively constant to larger temperatures due to the shell closure. Shown are also $N = 7$ and $N = 9$ which exhibit the large dips in the pairing strength in Fig. 2. They are generally below the neighboring even- N systems at low T , yet again confirming that the unpaired particle has a significant blocking effect on the pairing strength. Furthermore they have the same structure as the neighboring closed shell $N = 8$, but at lower magnitudes. It is also interesting to observe that, for $N = 7$ and 9 , the pairing strength is largest at finite T reflecting the competition between blocking by the unpaired particle and thermal excitations which moves the unpaired particle across the shell closure reducing the blocking effect. A similar effect has been found in SMMC studies for nuclei with odd nucleon numbers [30]. At higher T these effects are smoothed out as pairing vanishes and the pairing strength orders with increasing number of particles. Comparing the $g = 10$ and $g = 20$ results we see that the above effects are more pronounced for the stronger pairing strength and persists to higher temperature. This is consistent with the discussions above. Similar evidence for a transition at finite T in the homogeneous system in both energy and pair correlation was found in [24].

We have also considered the regime of $g < 10$ and found that at $g = 1$ (deep BCS regime) there are basically none of the interesting effects left. We therefore predict that for small systems with simple two-body pairing, there is a regime at $a > b$ where pairing features are pronounced. For $g > 20$ the calculation becomes unstable, so we cannot access this deep BEC regime.

In conclusion, the SMMC offers a good quantitative description of the behavior of equal mixtures of fermions in an interesting interaction regime. We studied the case of isotropic traps, and we extracted a number of particularly relevant properties. The excellent convergence properties of the method holds promise for application to specific situations where, e.g., deformation properties and formation of higher angular momentum pairs may become relevant. Deformation was studied in the nuclear case using the SMMC to predict shape transitions occurring as a function of temperature in the competition between pairing and quadrupole interactions [10]. This is relevant also for ultracold gases with the recent realiza-

tion of condensates with intrinsic long-range interactions between the atoms [32]. Recently the SMMC was also used to study the parity and spin properties of the density of states in nuclear systems [33, 34]. Transforming this to the atomic system could help us understand the low-energy excitation spectrum and the response of the gas to external perturbations.

The authors wish to thank A.S. Jensen, M. Thøgersen, and A. Juodagalvis for many fruitful discussions.

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- [1] K.M. O'hara *et al.*, Science **298**, 2179 (2002).
- [2] K. Dieckmann *et al.*, Phys. Rev. Lett. **89**, 203201 (2002).
- [3] C. Chin *et al.*, Science **305**, 1128 (2004).
- [4] M.W. Zwierlein *et al.*, Nature (London) **435**, 1047 (2005).
- [5] J. Kinast *et al.*, Science **307**, 1296 (2005).
- [6] J.T. Stewart, J.P. Gaebler, C.A. Regal, and D.S. Jin, Phys. Rev. Lett. **97**, 220406 (2006).
- [7] S. Jochim, private communication.
- [8] T. Stöferle, H. Moritz, K. Günter, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **96**, 030401 (2006).
- [9] C.W. Johnson, S.E. Koonin, G.H. Lang, and W.E. Ormand, Phys. Rev. Lett. **69**, 3157 (1992).
- [10] S.E. Koonin, D.J. Dean, and K. Langanke, Phys. Rep. **278**, 1 (1997).
- [11] D.J. Dean and M. Hjorth-Jensen, Rev. Mod. Phys. **75**, 607 (2003).
- [12] H. Heiselberg, Phys. Rev. A **68**, 053616 (2003).
- [13] S. Weinberg, Nucl. Phys. **B363**, 3 (1991).
- [14] H. Esbensen, G.F. Bertsch, and K. Hencken, Phys. Rev. C **56** 3054 (1997).
- [15] H. Heiselberg and B. Mottelson, Phys. Rev. Lett. **88**, 190401 (2002).
- [16] G.M. Bruun and H. Heiselberg, Phys. Rev. A **65**, 053407 (2002).
- [17] J. Carlson, S.Y. Chang, V.R. Pandharipande, and K.E. Schmidt, Phys. Rev. Lett. **91**, 050401 (2003).
- [18] S.Y. Chang and G.F. Bertsch, Phys. Rev. A **76**, 021603(R) (2007).
- [19] I. Stetcu, B.R. Barrett, U. van Kolck, and J.P. Vary, Phys. Rev. A **76**, 063613 (2007).
- [20] Y. Alhassid, G.F. Bertsch, and L. Fang, Phys. Rev. Lett. **100**, 230401 (2008).
- [21] F. Werner and Y. Castin, Phys. Rev. Lett. **97**, 150401 (2006).
- [22] F. Werner and Y. Castin, Phys. Rev. A **74**, 053604 (2006).
- [23] A. Bulgac, J.E. Drut, and P. Magierski, Phys. Rev. Lett. **96**, 090404 (2006).
- [24] V.K. Akkineni, D.M. Ceperley, and N. Trivedi, Phys. Rev. B **76** 165116 (2007).
- [25] J. von Stecher, C.H. Greene, and D. Blume, Phys. Rev. A **77**, 043619 (2008).
- [26] T. Busch, B.-G. Englert, K. Rzazewski, and M. Wilkens, Found. Phys. **28**, 549 (1998).
- [27] D.J. Dean, S.E. Koonin, K. Langanke, P.B. Radha, and Y. Alhassid, Phys. Rev. Lett. **74**, 2909 (1995).
- [28] K. Langanke, D.J. Dean, and W. Nazarewicz, Nucl. Phys.

- A757**, 360 (2005).
- [29] C. Özen, K. Langanke, G. Martínez-Pinedo, and D. J. Dean, Phys. Rev. C **75**, 064307 (2007).
 - [30] J. Engel, K. Langanke, and P. Vogel, Phys. Lett. **B429**, 215 (1998).
 - [31] E. L. Bolda, E. Tiesinga, and P. S. Julienne, Phys. Rev. A **66** 013403 (2002).
 - [32] Th. Lahaye *et al.*, Nature (London) **448**, 672 (2007).
 - [33] Y. Alhassid, S. Liu, and H. Nakada, Phys. Rev. Lett. **99**, 162504 (2007).
 - [34] Y. Kalmykov *et al.*, Phys. Rev. Lett. **99**, 202502 (2007).